where δ_{ij} is the Kronecker symbol; and the angle brackets denote the averaged by the volume Ω values: $<(...)>=(1/|\Omega|)\int_{\Omega}(...)d\Omega$.

These problems will be solved in a representative volume numerically by the finite element method.

3. Models of representative volumes

Finite element simulation of the representative volume Ω of the porous composite with closed porosity is based on the basic cubic cell Ω_c with the edge l_c. Along each edge the cell Ω_c is divided into three segments with the lengths a_p, l_p, a_p, where $l_c = l_p + 2a_p$, $l_p = k_p l_c$, $k_p < 1$. Thus, a basic cell is divided into 27 hexahedrals, which we initially assume to be dielectric finite elements. The center of the basic cell is the main (central) cubic finite element with the edge l_p. Then we translate the basic cell Ω_c n_c times by three coordinate axes and obtain an array of finite elements Ω by the size $L \times L \times L$ ($L = n_c l_c$), consisting of n_c^3 basic cells.

We assume that central finite elements inside basic cells can have material properties of pores. These "porous" finite elements are selected according to the following algorithm. We set a desired porosity p_s as a ratio of the desired volume of the pores to the total volume. Then the number N_p of central finite elements that can be pores will be determined according to the formula: $N_p = [p_s (n_c / k_p)^3]$, where [...] is the integer part of the number. We select these N_p central finite elements using a random number generator and then modify their material properties to the properties of pores. As a result, real porosity $p = N_p (k_p / n_c)^3$ will slightly differ from p_s. For example, with $n_c = 10$, $k_p = 0.8$ when p_s changes from 0.1 to 0.5 with the step 0.1 we have: $|p_s - p| \le 0.022$.

In order to simulate a partial metallization, we will assume that among six faces of "porous" finite element, two opposite faces, which are located perpendicular to one of the axial direction x_k, are electrodized. This direction x_k is chosen randomly for each "porous"element among the directions of three coordinate axes x_1, x_2 and x_3. Thus, in the representative volume Ω there will be N_p "porous" elements, which have $2N_p$ electrodized faces, where these paired faces are oriented randomly along the coordinate axes.

One of the cases of the volume Ω, built according to the described algorithm when $n_c = 10$, $k_p = 0.8$, $p_s = 0.1$, is given in Fig. 1. We note that the elements Ω_{pi} ($i = 1,2,...,N_p$) are randomly chosen among central elements of the cells, and therefore the next run of the algorithm changes their location (Fig. 1b). The choice of metallized surfaces (Fig. 1c) is not deterministic as well. Thus, the next run of the algorithm will also change the location of the generated surfaces Γ_{pi}, even in the case when the porous elements are the same.

In the result, we will obtain a representative volume of porous material with closed 3-0 porosity of partially stochastic structure. In this volume, there will be N_p elements-pores Ω_{pi}, all faces of which are in full contact with the boundaries of the neighboring elements of the composite material skeleton. Moreover, in each pore two opposite faces are assumed to be metallized.

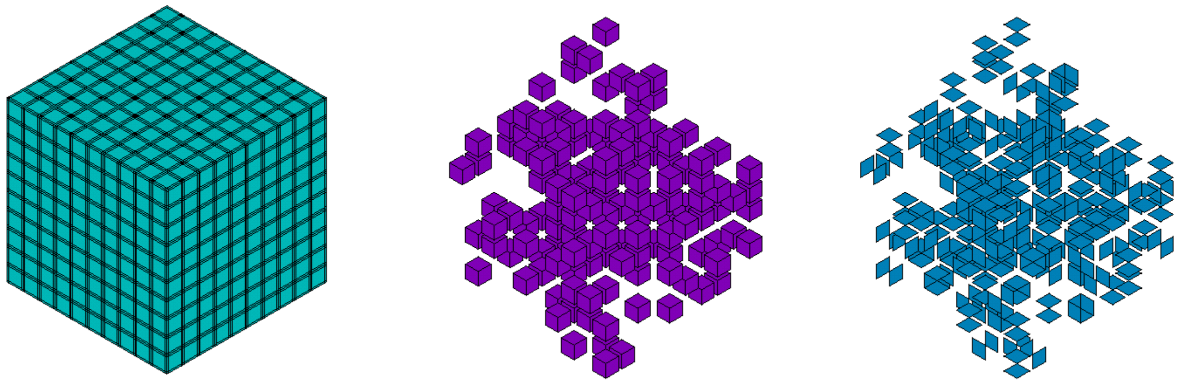


Fig. 1. Example of a representative volume: (*a*) whole volume, (*b*) porous elements, (*c*) metallized pore surfaces

4. Simulation of inhomogeneous polarization and finite element solution

A piezoceramic is a transversally isotropic material of 6*mm* class. Usually it is assumed to be homogeneously polarized in one direction (for example, along Ox_3-axis). For the polarization of a piezoceramic sample, it necessary to have process electrodes through which a strong electric field exceeding the coercive field can be applied. Thus, the polarization is defined not only by the material itself, but by geometry of the device as well. At microlevel, a porous piezoceramic is an inhomogeneous material Therefore, the polarization field around the pores can be inhomogeneous. Despite the fact that usually the effective properties of porous piezoceramic are defined in assumption of homogeneous polarization, some papers [23, 24] also investigated the influence of inhomogeneous polarization. As it has been shown in these papers, for small and average porosity this influence is rather small.

Obviously, for a porous piezoceramic with metallized pore surfaces, taking into account the inhomogeneity of the polarization field is more important. Indeed, the metallization of the pores is obtained by piezoceramic sintering, which is followed by the material polarization. It is clear that then the presence of conductive surfaces inside the material will additionally affect the distribution of the polarization field. In connection to this, in order to take into account inhomogeneous polarization of a porous piezoceramic around the pores, at the initial stage of the simulation we can model the process of polarization along Ox_3-axis. In order to do this, we solve a finite element problem of quasielectrostatic for a porous dielectric in a representative volume Ω, generated by the method described in the previous section.

Then, for the inhomogeneous cube Ω with the side L in Cartesian coordinate system $Ox_1x_2x_3$, we have the following boundary-value problem:

$$\nabla\cdot\mathbf{D}=0,\ \mathbf{D}=\boldsymbol{\varepsilon}\cdot\mathbf{E},\ \mathbf{E}=-\nabla\varphi,\ \mathbf{x}\in\Omega \qquad (12)$$

$$\varphi=V_j,\ \ \mathbf{x}\in\Gamma_{\varphi j},\ \ j=1,2;\ \mathbf{n}\cdot\mathbf{D}=0,\ \ \mathbf{x}\in\Gamma_q, \qquad (13)$$

where $\Gamma=\bigcup_j\Gamma_{\varphi j}\bigcup\Gamma_q$; $\Gamma_{\varphi j}$ are the electrodes $x_3=0$ and $x_3=L$; $\boldsymbol{\varepsilon}=\boldsymbol{\varepsilon}(\mathbf{x})$ is the matrix of dielectric permittivities of a nonpolarized ceramic with pores.

Problem (12), (13) should be supplemented by electric boundary conditions for pores from (5), (6). After solving the formulated problem, we can find the values of the polarization vectors $\mathbf{P}^{ek}=\mathbf{D}^{ek}-\varepsilon_0\mathbf{E}^{ek}$ in a central point of each finite element with the number k, which is not a pore. With these elements we associated their element coordinate systems $Ox_1^{ek}x_2^{ek}x_3^{ek}$, for which the axes Ox_3^{ek} were chosen such that their directions coincided with the directions of the polarization vectors $\mathbf{P}^{ek}$.

At the second stage, the finite elements of electrostatics were modified into the elements with possibilities of piezoelectric analysis. New elements were given material properties of two types, namely, the property of polarized piezoceramic for the elements of the material skeleton, and the negligibly small moduli for the pores. The finite elements of the skeleton were related to the element coordinate systems $Ox_1^{ek}x_2^{ek}x_3^{ek}$, defined by the polarization vectors $\mathbf{P}^{ek}$. Then, in order to determine the effective moduli, we solved the problems of electroelasticity (1)–(4) or (1)–(3), (5), (6) by the cases (7)–(11). We emphasize that with accounting for inhomogeneous polarization the problem of electroelasticity is solved for an inhomogeneous structure, where each finite element of the polarized piezoceramic has its own moduli $\mathbf{c}^{Eek}$, $\mathbf{e}^{ek}$, $\boldsymbol{\varepsilon}^{Sek}$, obtained by known formulas for recalculation of tensor components at the transfer from crystallographic Cartesian coordinate system $Ox_1x_2x_3$ to the element coordinate systems $Ox_1^{ek}x_2^{ek}x_3^{ek}$.

If we do not take inhomogeneous polarization into account, then problem (12), (13) is not used and in problem (1)–(4) or (1)–(3), (5), (6) all elements have either the properties of a piezoceramic material of 6*mm* class polarized along Ox_3-axis, or the properties of pores.

5. Numerical examples

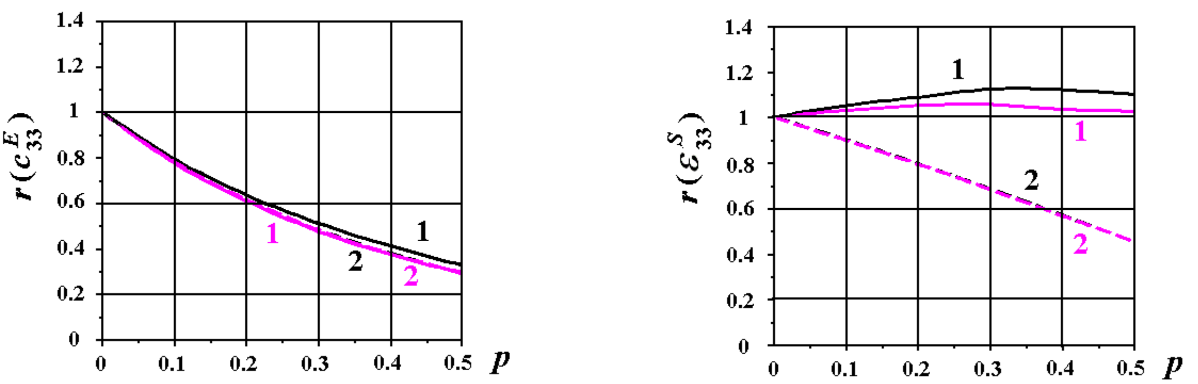
The homogenization problems were solved by the finite element method in ANSYS finite element package using the technique described above and in [23-25]. Special programs in ANSYS APDL were written for the representative volume generation, solution of the electrostatics problem (12), (13) and subsequent solution of five homogenization problems (1)–(4) or (1)–(3), (5), (6) with different boundary conditions (7)–(11). After solving the problems, the averaged characteristics were automatically calculated in ANSYS and thus the full set of the effective moduli was obtained. For the calculations, we used an eight-node finite element SOLID5 with the displacements and the electric potential as degrees of freedom in each node. For the problem of electrostatics, the option of only electric potential as degree of freedom was chosen. Numerical experiments were performed in ANSYS 11.0. However, the developed programs in ANSYS APDL will work in other versions of ANSYS that support piezoelectric analysis and finite element SOLID5.

To provide an example, we consider a porous pizoceramic PZT-4. For the dense piezoceramic PZT-4 we take the following values of material constants [27]: $c_{11}^E = 13.9\cdot 10^{10}$, $c_{12}^E = 7.78\cdot 10^{10}$, $c_{13}^E = 7.74\cdot 10^{10}$, $c_{33}^E = 11.5\cdot 10^{10}$, $c_{44}^E = 2.56\cdot 10^{10}$ (N/m^2); $e_{33} = 15.1$, $e_{31} = -5.2$, $e_{15} = 12.7$ (C/m^2); $\varepsilon_{11}^S = 730\varepsilon_0$, $\varepsilon_{33}^S = 635\varepsilon_0$. For the pores, we set negligibly small elastic moduli $c_{\alpha\beta}^{Ep} = \kappa c_{\alpha\beta}^E$, $\kappa = 10^{-10}$, piezomoduli $e_{i\alpha}^p = \kappa$ (x1 C/m^2) and $\varepsilon_{ii}^{Sp} = \varepsilon_0$. We consider a nonpolarized ceramic to be an isotropic material with the dielectric permittivity $\varepsilon = \varepsilon_{11}^S$. (a specific value of ε in the problem of electrostatics is not important, as the aim of this problem consists only in the determination of the polarization vector direction inside the composite material.) For the representative volume, we take the following geometric parameters: $L = 500$ (μm), $n_c = 10$, $k_p = 0.8$. In this case, the pores have the edges $l_p = k_pL/n_c = 40$ (μm).

We note that specific size L of the representative volume is not significant here, because we solve linear problem. On the contrary, the parameter n_c, which denotes the number of basic cells along coordinates axes, has great impact. It was verified that the chosen value $n_c = 10$ ensures the stability of the solution results under random generation of porosity for different launches of the program. The homogenized material has the same anisotropy class 6mm, as the initial material of piezoceramic PZT-4.

We will compare two model cases of the porous piezoceramics. In Case 1, we take into account the pore metallization by using the boundary conditions of free electrodes (5), (6). In Case 2, we consider ordinary porous piezoceramic, when only conditions (4) are held on the pore boundaries, and no equipotentiality conditions are satisfied on these boundaries. In addition, for each case we will consider the case of homogeneously polarized piezoceramic and the case of homogeneously polarized piezoceramic.

We are going to analyze the relative effective moduli. For example, $r(c^E_{\alpha\beta}) = c^{E\,\mathrm{eff}}_{\alpha\beta} / c^E_{\alpha\beta}$ are the values of the effective moduli $c^{E\,\mathrm{eff}}_{\alpha\beta}$, related to the corresponding values of the moduli $c^E_{\alpha\beta}$ for the dense piezoceramic, and so on. Also, we will use the index $l = 1, 2$ in more precise notation $r(c^E_{\alpha\beta})_l = (c^{E\,\mathrm{eff}}_{\alpha\beta})_l / c^E_{\alpha\beta}$ to denote the number of Case l, for which the moduli calculation was performed.



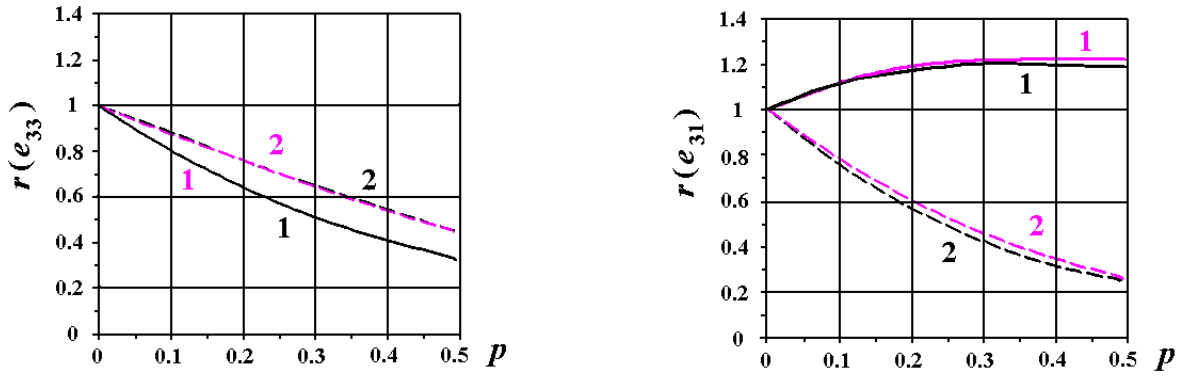
a) *b*)

Fig. 2. Dependencies of the effective elastic stiffness (*a*) and dielectric permittivity (*b*) on porosity

Typical behavior of the effective elastic stiffness moduli and the dielectric permittivity moduli are shown in Fig. 2 for the examples of the moduli $(c^{E\,\mathrm{eff}}_{33})_l$ and $(\varepsilon^{S\,\mathrm{eff}}_{33})_l$, $l = 1,2$. Here and after the black curves correspond to the case of inhomogeneously polarized piezoceramic and the magenta curves correspond to the case of the piezoceramic with homogenous polarization.

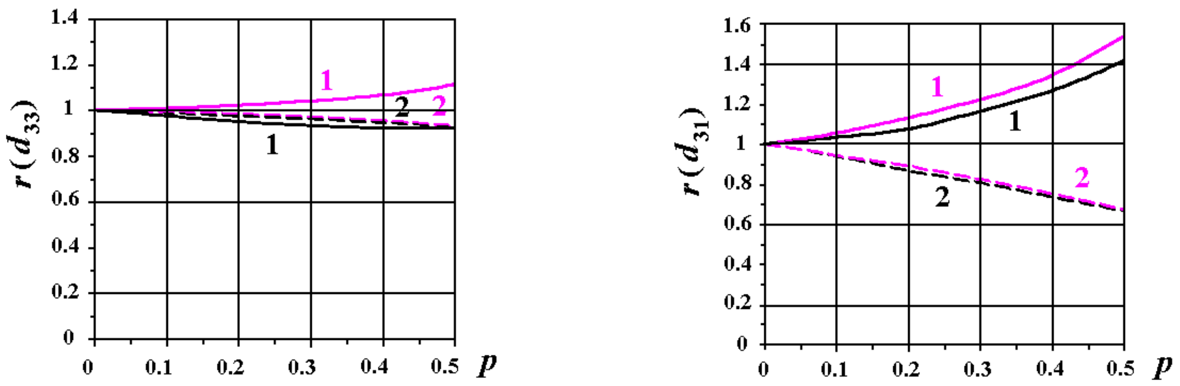
As it can be seen in Fig. 2a, the stiffness moduli decrease with the porosity growth in both cases, and the account for inhomogeneous polarization field has a weak effect on the stiffness moduli. Meanwhile (see Fig. 2b), the effective moduli of the dielectric permittivities decrease with the porosity growth (curves 2). However, the effective moduli of the dielectric permittivities for the porous piezoceramic with metallized pores increase when the porosity grows till $p = 0.3$ (curves 1), and this increase is stronger for the case of inhomogeneously polarized piezoceramic skeleton of the composite.

The piezomoduli behavior (Figs. 3, 4) is of more interest. For example, the piezomoduli $(e^{\mathrm{eff}}_{33})_2$ and $(e^{\mathrm{eff}}_{31})_2$ for ordinary porous piezoceramic decrease with the porosity growth. Meanwhile, for the piezoceramic with metallized pore surfaces the piezomodulus $(e_{33}^{\text{eff}})_1$ also decreases with the growth of p, and its decrease is faster than that of $(e_{33}^{\text{eff}})_2$. On the contrary, the piezomodulus $(e_{31}^{\text{eff}})_1$ grows when the porosity increases till $p = 0.3$, and then it gets stabilized or slightly decreases. Taking into account the inhomogeneous polarization does not influence the behavior of the piezomodulus e_{33}^{eff}, and for the piezomodulus e_{31}^{eff} it results in slightly greater decrease for the ordinary porous piezoceramic, and slightly greater increase for the porous piezoceramic with partial pore surface metallization.



a) *b*)

Fig. 3. Dependecies of the effective piezomoduli $r(e_{33})_l$ (*a*) and $r(e_{31})_l$ (*b*) on porosity



a) *b*)

Fig. 4. Dependecies of the effective piezomoduli $r(d_{33})_l$ (*a*) и $r(d_{31})_l$ (*b*) on porosity

For the piezomodulus $(d_{33}^{\text{eff}})_2$ of ordinary porous piezoceramic, its unusual property of a weak dependence on porosity is well known, however, the values of piezomodulus $(|d_{31}^{\text{eff}}|)_2$ decrease with the growth of p. As it can be seen from the curves 2 and 4, these properties are weakly dependent on the inhomogeneity of the polarization, whether it is taken into account or not.

For porous piezoceramic with metallized pore surfaces, as it can be seen in Fig. 4, the values of the piezomodulus $(|d_{31}^{\text{eff}}|)_1$ increase with the growth of p, and taking into account the inhomogeneity of polarization results in slightly less growth of the piezomodulus $(|d_{31}^{\text{eff}}|)_1$ in its absolute value. The piezomodulus $(d_{33}^{\text{eff}})_1$, with taking the inhomogeneous polarization into account, almost does not change with the porosity growth, i. e. it behaves in the same manner as for ordinary porous piezoceramic. If we consider the piezoceramic material of the composite to be homogeneously polarized, then the piezomodulus $(d_{33}^{\text{eff}})_1$ will also increase with the growth of porosity. Thus, we can conclude, that taking into account the inhomogeneity of polarization for the piezoceramic material with partially metallized pore surfaces has a significant influence on the values of the piezomoduli d_{3j}^{eff}.

6. Conclusions

In the present work, the properties of the inhomogeneously polarized porous piezoceramic with partially metallized pore surfaces have been investigated with the help of the methods of the composite mechanics and mathematical modelling. The pore surface metallization has been taken into account only by the electric boundary conditions of equipotentiality. The results of the numerical experiments have shown that microporous piezoceramic with metallized pore surfaces has a range of unusual properties, which are perspective for practical applications [28]. The comparison of the obtained results with similar results provided in [23, 24] for the case of full pore surface metallization has shown that partial metallization slightly eliminates unusual properties of the effective moduli [25]. The computation results showed that taking into account the inhomogeneity of the polarization field of the composite material was more significant for the determination the effective values of piezomoduli and dielectric permittivities, and less important for the determination of the effective elastic stiffness moduli.

We would like to note, that the developed model of the representative volume has only partially random porosity structure, as there are domains with the thickness $2a_p$ or a_p, which go through the whole volume and do not contain pores. In connection to this, the patterns of the inhomogeneous polarization field influence can be different for other internal structures of the representative volumes. Also, the values of the effective moduli are influenced by the extent of the pore surface metallization and the thickness of the metallized covering, which was noted in [24] for the case of homogeneously polarized piezoceramic.

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